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CALIFORNIA INSTITUTE OF TECHNOLOGY

DYNAMIC PROPERTIES LABORATORY

A Comparison Between Dislocation Theory and Experimental Measurements of Delayed Yield in Steel

by

T. Vreeland, Jr. and D. S. Wood

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April 1954

A COMPARISON BETWEEN DISLOCATION THEORY

AND

EXPERIMENTAL MEASUREMENTS OF DELAYED YIELD IN STEEL

By

T. Vreeland, Jr. and D. S. Wood

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A COMPARISON BETWEEN DISLOCATION THEORY AND EXPERIMENTAL MEASUREMENTS OF DELAYED YIELD IN STEEL

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ABSTRACT

A dislocation model of a yield nucleus for materials, such as annealed low-carbon steel, which exhibit a distinct yield point, is presented. On the basis of the model an analytical expression is derived which relates the time delay for yielding under constant applied stress to the magnitude of the stress and the temperature. This expression involves the ratio of the binding energy of a dislocation with a Cottrell "atmosphere" to the total energy of a dislocation. The expression also involves the frequency of thermal fluctuations associated with the release of a dislocation from an "atmosphere". The numerical values of these two constants are chosen to fit the analytical expression to experimental data. The value of the ratio of the binding energy to the total energy so determined is essentially the same as the value obtained by Fisher (1)*. However, this value disagrees markedly with the theoretical estimate made by Cottrell (3). The value of the frequency of thermal fluctuations is shown to be in substantial agreement with the frequency to be expected from consideration of the length of the thermally activated portion of a dislocation during the process of its release from an "atmosphere".

* The figures appearing in parentheses pertain to the references appended to this report.

INTRODUCTION

A Theory of the delay time for the initiation of yielding in materials which exhibit a distinct yield point has been recently proposed by J. C. Fisher (1). This theory is based upon a relatively simple dislocation model and predicts the dependence of the delay time for yielding at constant stress upon the stress and temperature. The results of the theory were compared with experimental measurements (2) of the delay time for yielding at constant stress in annealed mild steel as a function of stress and temperature.

One of the adjustable constants used to fit the experimental data is essentially the frequency factor associated with the thermally activated process involved. The other constant is a function of the ratio of the binding energy between a dislocation and an "atmosphere" of interstitial solute atoms to the total energy of a dislocation without an "atmosphere". The value of this energy ratio which Fisher finds by fitting his theoretical formula to the delay time data is about 1/3 per cent. Several methods of estimating the binding energy based upon both theoretical considerations and experimental evidence have been discussed by Cottrell (3). They all indicate a value of approximately 0.5 eV per atomic distance along the dislocation line. Since the energy of an unanchored dislocation is generally estimated to be approximately 5 eV per atomic distance, the expected energy ratio is about 10 per cent rather than 1/3 per cent.

The purpose of this report is to analyze a more complex dislocation model than that used by Fisher to determine if by means of such a model results can be obtained that are more in accord with the theoretical value of the binding energy discussed above.

DISLOCATION MODEL OF A YIELD NUCLEUS

The dislocation model of a yield nucleus employed in this report has been discussed previously (2), (4). Briefly, this model consists of a slip surface bounded by a grain boundary and containing a Frank-Read dislocation source (5) (a short segment of dislocation line with fixed end points). The source dislocation is assumed to have associated with it a Cottrell "atmosphere" (6) of interstitial solute atoms such as carbon and nitrogen. Dislocation loops are generated at the Frank-Read source when a stress is applied. The first of these expands rapidly outward from the source until it is held up by the grain boundary, as Cottrell has suggested (7). Succeeding dislocation loops expand until they reach equilibrium configurations between the source and the first dislocation. The inhomogeneous stress fields of the dislocations which accumulate in the slip surface in this manner are added to the applied stress. This results in two important effects. First, the local stress at the grain boundary increases as the number of accumulated dislocations increases. Macroscopic yielding is assumed to begin when this stress reaches a critical value. Second, the local stress at the Frank-Read source decreases as the number of accumulated dislocations increases. This results in a decrease in the rate of generation of new dislocations during the delay period prior to the onset of macroscopic yielding.

A polycrystalline specimen of low-carbon steel is assumed to contain many such yield nuclei. Those nuclei which are favorably oriented with respect to an applied stress are the source of the inelastic microstrains which are observed to occur prior to the beginning of macroscopic yielding (4), (8). Yielding is initiated at the site of the nucleus which first produces the critical grain boundary stress. Thus the delay time for yielding under constant applied stress is governed by the properties of this most critical nucleus. This is a nucleus which is so oriented that it is subjected to the maximum possible resolved shear stress, namely, one half the value of an applied tensile stress. Also, as will appear later, it is a nucleus in which the distance from the Frank-Read source to the grain boundary is a maximum. Thus yielding is initiated, according to this

model, in one of the largest grains of the specimen, and by a dislocation source which lies near the center of the grain.

This dislocation model for the initiation of yielding differs from that discussed by Fisher (1) in two respects. First, the critical condition for the onset of yielding depends upon the magnitude of the applied stress as well as the number of dislocations generated by the Frank-Read source, whereas Fisher assumes only the latter. Second, the rate of generation of dislocations decreases, under constant applied stress, as the number generated increases. Fisher assumes that the rate of generation is constant.

THEORY OF THE DELAY TIME FOR YIELDING UNDER CONSTANT APPLIED STRESS

An expression for the delay time for yielding under constant applied stress as a function of stress and temperature may be derived in the following manner on the basis of the dislocation model of a yield nucleus described above. The rate of generation of dislocation loops at the Frank-Read source is assumed to be controlled by the thermally activated release of the source dislocation from its "atmosphere" in a manner similar to that described by Cottrell and Bilby (9). Fisher (1) has proposed a simpler expression for the activation energy than that derived by Cottrell and Bilby. Although Fisher's expression involves a somewhat greater degree of approximation than the Cottrell-Bilby relation, the former expression will be used in this report, namely:

$$W = \frac{\gamma_o^2}{b\tau_s} f\left(\frac{\gamma}{\gamma_o}\right) \qquad (1)$$

where
$$f\left(\frac{\gamma}{\gamma_o}\right) = \cos^{-1}\left(\frac{\gamma}{\gamma_o}\right) - \frac{\gamma}{\gamma_o}\left(1 - \frac{\gamma^2}{\gamma_o^2}\right)^{\frac{1}{2}},$$

γ_o is the energy per atomic distance of a dislocation without an "atmosphere",

γ is the energy per atomic distance of a dislocation with an "atmosphere",

b is the atomic slip distance or Burgers vector,

and τ_s is the resolved shear stress at the Frank-Read source.

Although the source dislocation may be released from its atmosphere when the energy given by equation 1 is supplied by a thermal fluctuation, a new dislocation loop will not be generated unless

$$\tau_s \geq \frac{Gb}{\ell} \qquad (2)$$

where G is the shear modulus,

and ℓ is the distance between the end points of the Frank-Read source.

Equation … dition that the stress must be capable of extending t… dislocation out into a semicircular arc.

Thus … tion of dislocation loops is given by

$$\dot{n} = \nu \qquad \tau_s \geq \frac{Gb}{l} \tag{3}$$

$$\dot{n} = 0 \qquad \cdot \; \frac{Gb}{l}$$

where n is … tions generated,

ν is the … ropriate form of thermal fluctuati…

k is Boltzman's constant,

and T is the absolute temperature.

Now it is necessary to relate the local resol… shear stress at the Frank-Read source to the applied stress and the num… of dislocations generated. Such a relation has been previously derived (4) … a consideration of the equilibrium configuration of a planar array of straight dislocations acted upon by an applied stress and with the first dislocation held up at a grain boundary. This relation is

$$n = \frac{L}{B}\left(\tau_a - \tau_s^2/\tau_a\right), \quad \tau_a \geq \frac{Gb}{l}$$

$$n = 0 \qquad\qquad , \quad \tau_a < \frac{Gb}{l} \tag{4}$$

where L is one half the shortest distance along the slip surface from the source to the grain boundary,

$B = \frac{Gb}{2\pi}$

and τ_a is the applied resolved shear stress.

Equation 4 is only applicable to those sources which are located at such positions within a grain that L is much less than the grain diameter. The largest number of dislocations will be generated by a source which lies at or near the center of a large grain (maximum value of L). Such a source will govern the initiation of yielding. Hence equation 4 requires modification for use in the present analysis. An approximate modification may be deduced from the work of Leibfried (10) and gives

$$n = \frac{L}{\pi B}\left(\tau_a - \tau_s^2/\tau_a\right) \quad , \quad \tau_a \geq \frac{Gb}{\ell}$$
$$n = 0 \quad , \quad \tau_a < \frac{Gb}{\ell}. \qquad (5)$$

Equation 5 applies to an antisymmetric arrangement of straight parallel dislocations with the source dislocation in the center and arrays of dislocations of apposite sign on either side of it. This is assumed to represent a sufficiently good approximation to the present case of concentric circular dislocations with the source in the center. The value of the shear stress at the Frank-Read source according to equation 5 is

$$\tau_s = \tau_a\left(1 - \frac{\pi n B}{\tau_a L}\right)^{\frac{1}{2}}, \qquad (6)$$

The local resolved shear stress at the grain boundary is also a function of both the applied stress and the number of dislocations accumulated in the yield nucleus. This stress is assumed to be the same as the stress at a single locked dislocation which is obstructing the motion of an array of n linear dislocations. An expression for this stress has been given by Eshelby, Frank, and Nabarro (11), namely

$$\tau_b = n\,\tau_a \qquad (7)$$

where τ_b is the local resolved shear stress at the grain boundary.

If the critical value of τ_b at which dislocations break through or are generated at the grain boundary is $\tau_b{}^*$, then yielding begins when the number of dislocations accumulated in the yield nucleus reaches the value

$$n^* = \tau_b^*/\tau_a\,. \qquad (8)$$

However, in view of equation 3 this number of dislocations can be generated only if

$$\tau_s \geq \frac{Gb}{\ell}$$

throughout the yield delay period. Thus, using equation 6, the minimum value of the applied stress which can cause yielding (i.e. the resolved static upper yield shear stress) is

$$\tau_y = \left\{ \left(\frac{Gb}{\ell}\right)^2 + \frac{\pi B \tau_b^*}{L} \right\}^{\frac{1}{2}}. \tag{9}$$

For applied stresses $\tau_a \geq \tau_y$, yielding will occur in the time required to generate n^* dislocations. From equation 3 this time is

$$t_d = \frac{1}{\nu} \int_{n=0}^{n=n^*} \exp\left(\frac{W}{kT}\right) dn \, . \tag{10}$$

Using equations 1, 6, and 8 in equation 10 the final expression for the yield delay time becomes

$$t_d = \frac{1}{\nu} \int_{n=0}^{n=\tau_b^*/\tau_a} \exp\left[\frac{\gamma_0^2 f\left(\frac{\gamma}{\gamma_0}\right)}{\tau_a b kT \left(1 - n\pi B/\tau_a L\right)^{\frac{1}{2}}}\right] dn \quad \text{for } \tau_a \geq \tau_y, \tag{11}$$

$$t_d = \infty \qquad \text{for } \tau_a < \tau_y \, .$$

COMPARISON OF THEORY AND EXPERIMENT

The results of the theory as represented by equation 11 may be compared with experimental measurements (2) of the delay time for yielding in an annealed low-carbon steel as a function of applied stress and temperature. The various constants in the theory are chosen as follows:

(a) $G = (13.30 - 0.003T) \times 10^6 \ \mathrm{lb/in.^2}$, where T is the absolute temperature in degrees Kelvin. This is based upon Köster's measurements (12) of Young's modulus and the assumption that Poisson's ratio is independent of temperature.

(b) $b = 0.985 \times 10^{-8} \ \mathrm{in.}$ is the Burgers vector for iron.

(c) $\gamma_0 = \dfrac{Gb^2}{2}$ is the usual type of expression for the energy of a dislocation and gives about 4.2 electron volts per atomic plane along the dislocation.

(d) $L = 1.1 \times 10^{-3} \ \mathrm{in.}$ is based upon the assumption that the largest grain in the material has about three times the diameter of the average grain.

(e) $\tau_b^* = \dfrac{G}{2\pi}$ is equal to the theoretical strength of a perfect crystal lattice.

(f) $\ell = 680\, b$ is the value of ℓ which provides agreement between equation 9 and the value of the static upper yield stress at room temperature which was determined experimentally. This value of ℓ also agrees approximately with values deduced from measurements of pre-yield inelastic microstrains (4).

(g) $\nu = 6.77 \times 10^{10}\ sec^{-1}$ is the value which is found to provide the best fit between equation 11 and the experimental data.

(h) $\left(1 - \frac{\gamma}{\gamma_o}\right) = 0.0037$ is the value found to provide a good fit with the experimental data.

The values of the applied resolved shear stress, τ_a, are taken to be one-half the values of the applied tensile stress employed in the experiments.

The calculations of the integral in equation 11 were made by means of an asymptotic expansion. A sufficient number of terms of the expansion were retained to give a maximum uncertainty of 0.1 in the calculated values of the logarithm of the delay time in seconds. The solid lines in Fig. 1 indicate the numerical results of these calculations while the plotted points represent the experimental data.

The theory may also be compared with experiment in another respect. Values of the initial microstrain rate when stress was first applied may be obtained from the experimental measurements of pre-yield inelastic microstrains (4). The logarithms of these values in sec^{-1} units are plotted in Fig. 2 versus the reciprocal of the applied tensile stress. These data were obtained at a temperature of 73°F (296°K). A straight line is drawn to represent the average trend of the data. If it is assumed that this microstrain rate is proportional to the rate of generation of dislocation loops in yield nuclei, then the theoretical value of the slope of the line in Fig. 2 may be obtained approximately from equations 1 and 3. Assuming that at the initial instant of load application the microstrain rate is governed by the maximum resolved shear stress, then $\tau_s = \tau_{a\,max.} = \sigma/2$,

and hence
$$\frac{d\left(\log_{10} \dot{\varepsilon}\right)}{d\left(\frac{1}{\sigma}\right)} = -\frac{2\gamma_o^2 f\left(\frac{\gamma}{\gamma_o}\right) \log_{10} e}{bkT} . \qquad (12)$$

When equation 12 is fitted to the line in Fig. 2 the value

$$\left(1 - \frac{\gamma}{\gamma_o}\right) = 0.0015$$

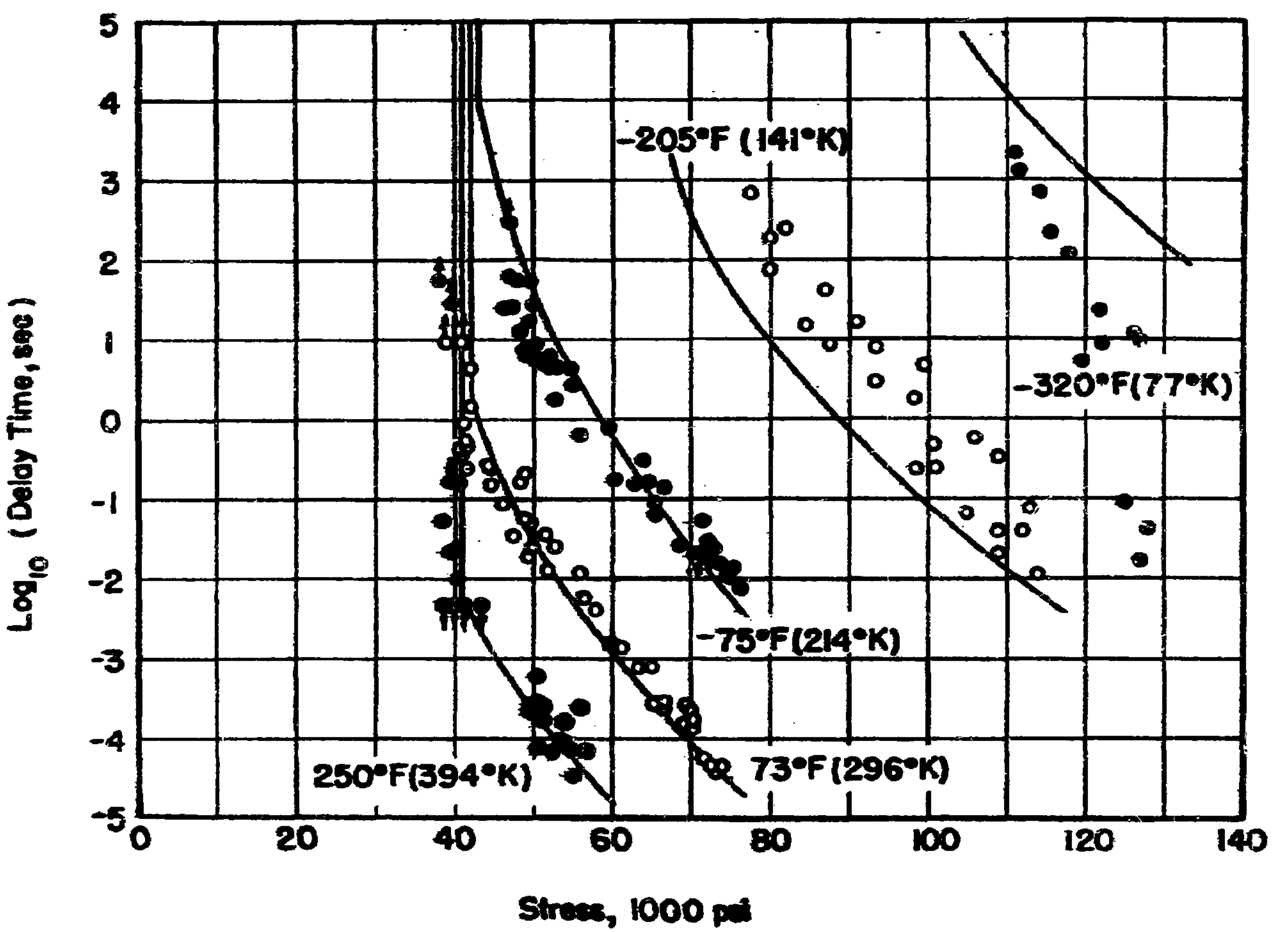

Fig. 1 Logarithm of the Delay Time vs. the Tensile Stress for an Annealed 0.17% Carbon Steel at Five Temperatures from -320°F (77°K) to 250°F (394°K).

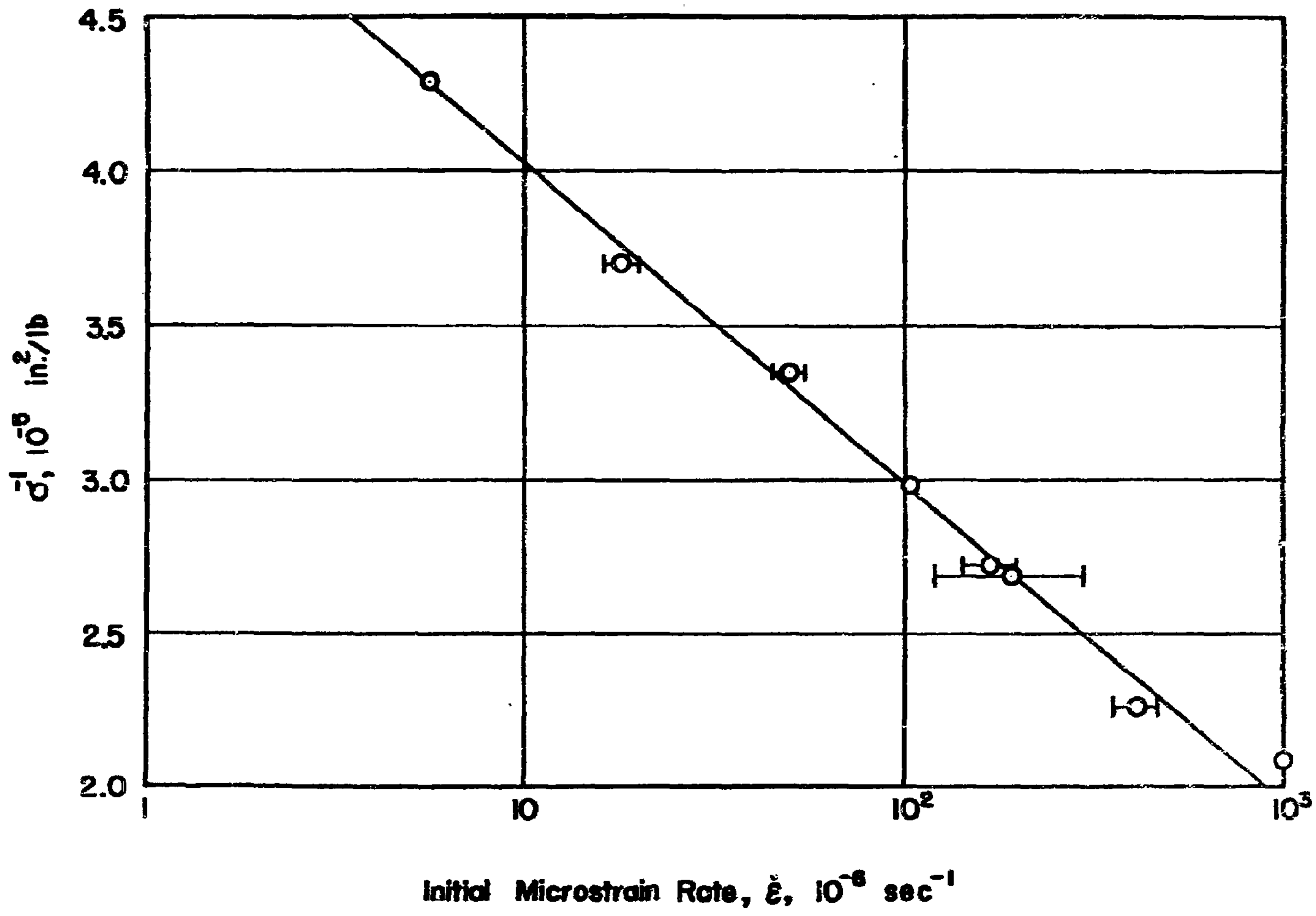

Fig. 2 Reciprocal of the Tensile Stress vs. the Initial Microstrain Rate for an Annealed 0.12% Carbon Steel at 73°F (296°K).

is obtained for the ratio of the binding energy of a dislocation with a Cottrell "atmosphere" to the total energy of the dislocation. This value compares favorably with that which was found to give a good fit of equation 11 to experimental data, considering the various approximations involved.

DISCUSSION OF RESULTS

The values of the energy ratio, $\left(1-\frac{\gamma}{\gamma_0}\right)$ obtained in this investigation are substantially the same as the value obtained by Fisher (1), namely a few tenths of one per cent.

A few attempts to employ other reasonable values of the constants τ_b^* and L which appear in the theory have been made. These modifications tend to give a poorer fit with the experimental data without leading to an appreciable increase in the value of the energy ratio.

Thus the more complex dislocation model employed in the present report does not resolve the discrepancy between the energy ratio found by Fisher and the theoretical value which is estimated by Cottrell (3) to be about ten per cent. The essential difference between theory and experiment in this respect is that the theory (for the binding energy) predicts a much greater sensitivity of the yield delay time to temperature changes than is observed experimentally. A major revision of some aspect of the theory may be required to resolve the discrepancy.

The differences between the theory and experimental data for a temperature of -205°F (141°K) indicated in Fig. 1 might be attributed to the use of an incorrect value of the shear modulus at that temperature. An increase of ten per cent over the value used would improve the fit considerably. The authors are aware of no measurements of the shear modulus of iron or steel at temperatures in this range. The discrepancy between theory and experiment at -320°F (77°K) may be associated with some change in the mechanism of yielding. This is suggested by the occurrence of brittle fractures after little or no plastic deformation in the tests made at -320°F.

The value of the frequency, ν, of the thermal fluctuations for release of the source dislocation from its atmosphere which is found by fitting the theory to experimental measurements of yield delay times appears to be a reasonable value, as the following considerations indicate. The length of the activated portion of the source dislocation at the time of its release from the "atmosphere" may be estimated as follows. The radius

of curvature of the activated section of dislocation is $\frac{\gamma_0}{\tau_s b}$. Numerically this gives a radius of curvature of about 250 b , when $\tau_s = 25 \times 10^3$ lb/in.^{2} which is within the lower range of experimental stresses. From the work of Cottrell and Bilby (9) it appears reasonable to assume that the center of the activated segment of dislocation moves a distance of about 4 b away from the "atmosphere". These values lead to a length of the activated segment of the source dislocation of about 0.9×10^{-6} in. The wave length of a thermal fluctuation causing this segment of dislocation to be activated is thus about 1.8×10^{-6} in. Since the velocity of shear waves in iron is about 1.3×10^5 inches per second, the above wave length corresponds to a frequency of 7.2×10^{10} cycles per second. The latter value agrees well with the value obtained by selecting the constants of the theory to fit the yield delay time data.

Further consideration of the thermally activated length of the "anchored" dislocation indicates that the frequency, ν , is approximately proportional to the square root of the local stress at the dislocation source, τ_s . Some modification of the theory given in this report would be required to take this effect into account. However, such a modification would probably have only a small effect on the final result of the theory.

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